

Model Performance

Model	Data
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Weighted KNN model

5-fold CV (75%)		Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE
0.85	1.14	0.85	1.12	0.83	1.23

## Model Results

**Predicted value:**  $4.19\text{e-}13 \text{ cm}^3/\text{molecule}\cdot\text{sec}$

**Global applicability domain:** Inside

**Local applicability domain index:**  $6.41\text{e-}01$

**Confidence level:**  $4.97\text{e-}01$

## Nearest Neighbors from the Training Set

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Cyclopropane

**Measured:**  $8.40\text{e-}14$

**Predicted:**  $4.19\text{e-}13$

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Cyclobutane

**Measured:**  $1.50\text{e-}12$

**Predicted:**  $1.78\text{e-}12$

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Cyclopentane

**Measured:**  $5.16\text{e-}12$

**Predicted:**  $6.13\text{e-}12$

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Methanethiol

**Measured:**  $3.29\text{e-}11$

**Predicted:**  $1.37\text{e-}11$

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Cyclohexane

**Measured:**  $7.49\text{e-}12$

**Predicted:**  $7.04\text{e-}12$